A variational problem on the probability simplex

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Abstract—We investigate a variational problem on the probability simplex with a path cost expressed as a sum of two terms reminiscent of Lagrangian mechanics. This arose first in a 1972 paper of Y. M. Svirezhev on mathematical genetics, where it was demonstrated that solutions to certain equations governing evolutionary processes are extremals of the variational problem. In the present work, we show that this result holds generally for replicator dynamics, a natural class of dynamical systems on the probability simplex, of great interest in evolutionary game theory. The Lagrangian of Svirezhev respects time-translation symmetry and hence has a conserved quantity, the energy. In particular, solutions to replicator dynamics are extremals confined to the zero level set of energy. Solutions of the dual Hamiltonian system are also of interest. Here we investigate their properties in relation to 2 x 2 matrix games, and assert existence of periodic orbits under suitable hypotheses.

I. INTRODUCTION

The question central to this work is the following: what do the natural selection equations or replicator dynamics optimize? Two principles answering this question are well known in mathematical genetics. Fisher's fundamental theorem of natural (Darwinian) selection states that the mean fitness of a population of finite number of types, each with a fitness linearly dependent on the population proportions (or frequencies), increases along the solutions of the selection equations. This can be shown by computing the gradient of the mean fitness using a natural Riemannian metric on the simplex, namely the Fisher-Rao-Shahshahani metric (defined below in section I.B), to yield the appropriate selection equations. While this statement is also true when the fitness is frequency independent as shown in [1], it is not true for a general nonlinear fitness. Kimura's maximum principle states that the increase in mean fitness is highest along solutions to the selection equations, compared to other simplex-preserving dynamics [2]. See also [3] for related discussions.

As reported in subsequent works such as [4]–[6], in his 1972 work, Svirezhev [7] showed that a cost functional given as the sum of the geodesic path length and the variance of a fitness integrated over a small enough time duration is minimized by *certain instances* of replicator dynamics, and that any simplex-preserving dynamics which can be written as a gradient dynamics is a candidate minimizer for the cost (discussed in detail in [8]). This theorem also finds mention

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in the work by Schoemaker [9] in a broader discussion of optimality as a heuristic, particularly in the commentary by James F. Crow. In what follows, to keep this paper somewhat self-contained, we describe certain concepts and notations from mathematical genetics and evolutionary game theory.

A. The replicator dynamics

Consider a large population of individuals falling into n types. Let $\Delta^{n-1} = \left\{x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}_+^n \middle| \sum_k x_k = 1\right\}$ denote the n-1 dimensional probability simplex, with x_i denoting the probability or relative frequency of type i, $i=1,\ldots,n$ and \mathbb{R}_+^n the positive orthant. Let $f(x) = [f^1(x) \ f^2(x) \ \ldots \ f^n(x)]^T$ denote the fitness map, a vector composed of fitness of the n types, dependent on the state x on the simplex. The replicator dynamics on Δ^{n-1} are selection equations that describe the evolution of the frequencies of the types according to the set of ordinary differential equations:

$$\dot{x}_i = x_i \left(f^i - \bar{f} \right) , \quad i = 1, \dots, n \tag{1}$$

where $\bar{f} = \sum_k x_k f^k(x)$ is the average fitness. It can be verified that $\sum_k \dot{x}_k = 0$, and that $x_k(t_0) = 0 \implies x_k(t) = 0 \ \forall \ t > t_0$, ensuring the preservation of the simplex. These equations can be interpreted as the o.d.e limit of discrete-time probability update equations:

$$x_k(t+1) = \frac{f^k}{\bar{f}} x_k(t) \tag{2}$$

as shown in [3], [10], under the assumption that \bar{f} does not change sign. The logarithmic growth rate of each type $\frac{\dot{x}_i}{x_i}$ is determined by how the fitness $f^i(x)$ of type i fares in comparison with the average fitness $\bar{f}(x)$, when the population is in state x. The replicator equations do not allow mutations since $x_i = 0 \implies \dot{x}_i = 0$. Therefore, if a type is extinguished, it remains extinguished for all future time leaving the sub-simplices of Δ^{n-1} positively invariant.

Interpreting a type in the setting of population genetics to refer to an allele constituting a genotype, we summarize three kinds of processes that govern the abundance of the alleles: (i) Selection: Suppose that w_{ij} denotes the constant fitness of a genotype comprising a pair of alleles i and j in a single population of n alleles. Assuming random mating of the types, the deterministic dynamics of selection is exactly (1) with fitness f(x) = Wx, $W = [w_{ij}]$, $1 \le i, j \le n$ satisfying $W = W^T$.

(ii) Mutation: Allowing for mutations of the types and denoting ε_{ij} to be the mutation rate from type j to i, with

 $\varepsilon_{ij} \ge 0$, $\sum_i \varepsilon_{ij} = 1$, the mutation equations in the absence of selection are given by

$$\dot{x}_i = \sum_{j=1}^n \varepsilon_{ij} x_j - x_i \tag{3}$$

(iii) Migration: Migration equations model the effect of an inflow of genotypes from a large migrant population whose frequencies q_i of types i = 1, ..., n are constant:

$$\dot{x}_i = q_i - x_i \tag{4}$$

Writing down the solution to the linear equations (4) leads one to observe that x = q is a globally exponentially stable equilibrium point for this dynamics.

B. Riemannian geometry of the simplex

Due to the work of Shahshahani [11] and Svirezhev [8], it is known that one can view the three dynamics, suitably restricted, as gradient dynamics. To see this, one needs to consider the simplex as a Riemannian manifold with boundary, equipped with the Fisher-Rao-Shahshahani (FRS) metric $G = [g_{ij}]$ where $g_{ij} = \delta_{ij} \frac{1}{x_i}$, $1 \le i, j \le n$ well defined in its interior [3]. Let $T_x \Delta^{n-1}$ denote the tangent space to the simplex at x. This is an n-1 dimensional vector space with vectors whose components sum to zero. We denote the FRS inner product of tangent vector u, v evaluated at x to be $\langle u, v \rangle_{FRS} = \sum_k \frac{u_k v_k}{x_k}$. When the fitness f(x) is either frequency independent or linearly dependent on the frequencies as encountered in population genetics, the replicator dynamics is the gradient with respect to the FRS metric of the mean fitness \bar{f} , upto a constant scaling factor. This is known as Fisher's fundamental theorem of natural selection. The migration dynamics is a negative gradient of the Kullback-Leibler divergence measure $D_{KL}(q||x) = \sum_{k} q_k \log \frac{q_k}{x_k}$. Additionally, when the mutation parameters in (3) satisfy

$$\varepsilon_{ij} = \begin{cases} \varepsilon_i, & i \neq j \\ 1 + \varepsilon_i - \varepsilon, & i = j \end{cases}$$
 (5)

where $\varepsilon = \sum_k \varepsilon_k$, (3) is a variant of the migration equations with $x_i = \frac{\varepsilon_i}{\varepsilon}$, i = 1, ..., n being the globally exponentially stable equilibrium and hence under these conditions, (3) is also a gradient dynamics. We refer the reader to [12] and references therein for a complete treatment of this topic. Although mutation and migration equations are not readily of the form of replicator dynamics, both can be rewritten to obtain a suitable fitness for which (1) holds in the interior of the simplex [13].

C. Structure of this paper

We formulate the minimization problem in section II, show that Svirezhev's result holds true for a general fitness (Theorem 2.1) and lay the groundwork for the Hamiltonian viewpoint to follow. In section III, the time-invariance of the Lagrangian for the problem posed by Svirezhev allows us to define a conserved quantity, the energy. We show that replicator dynamics live on the zero level set of energy. We state a theorem on the existence of periodic orbits as

solutions to Hamilton's equations. These results are stated for dynamics on the phase space of the one dimensional simplex in section IV and illustrated through a numerical example in section V, with concluding remarks in section VI.

II. PROBLEM FORMULATION

Our goal is to find trajectories on the simplex that minimize the cost functional J:

$$J = \int_{t_0}^{t_1} \sum_{k=1}^{n} \left[\frac{\dot{x}_k^2}{x_k} + x_k \left(f^k(x) - \bar{f} \right)^2 \right] dt \tag{6}$$

The cost comprises a velocity dependent term $T(x,\dot{x})$ and a position dependent term V(x) defined as:

$$T(x,\dot{x}) = \sum_{k=1}^{n} \frac{\dot{x}_{k}^{2}}{x_{k}} = ||\dot{x}||_{FRS}^{2},$$

$$V(x) = -\sum_{k=1}^{n} x_{k} \left(f^{k}(x) - \bar{f}(x) \right)^{2}$$
(7)

interpreted respectively to be analogues of kinetic and potential energy in mechanics. Svirezhev [8] showed that the aforementioned cost functional with linear fitness map given by f(x) = Wx, $W = [w_{ij}], 1 \le i, j \le n$ is minimized for trajectories in the simplex determined by natural selection, assuming that $t_1 - t_0$ is small enough. In addition, he noted that the same conclusions hold for the mutation and migration equations. The locality of this result should be noted here. Stating a similar result for longer time intervals would require analysis using conjugate point theory, beyond Legendre's second order condition, as used by Svirezhev. We prove below that the result of Svirezhev holds for a general fitness map, i.e., solutions to replicator dynamics are extremals of J.

Theorem 2.1. Let $x \in \Delta^{n-1}$. The replicator dynamics defined by the fitness $f(x) = [f^1(x) \dots f^n(x)]^T$:

$$\dot{x}_i = x_i \left(f^i - \bar{f} \right) \quad i = 1, \dots, n \tag{8}$$

satisfies the Euler-Lagrange equations associated with extremizing the following cost functional in the interior of the simplex:

$$J = \int_{t_0}^{t_1} \sum_{k=1}^{n} \left(\frac{\dot{x}_k^2}{x_k} + x_k \left(f^k - \bar{f} \right)^2 \right) dt \tag{9}$$

Proof. We have an extremization problem with the holonomic simplex constraint. Therefore, consider the Lagrangian $\mathscr L$ with Lagrange multiplier λ for this cost functional:

$$\mathcal{L} = \sum_{k=1}^{n} \left(\frac{\dot{x}_k^2}{x_k} + x_k \left(f^k - \bar{f} \right)^2 + \lambda x_k \right) - \lambda \tag{10}$$

Then, the associated Euler-Lagrange equations are given by:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_i} = \frac{\partial \mathcal{L}}{\partial x_i} \tag{11}$$

Calculating each term separately, we get:

$$\frac{\partial \mathcal{L}}{\partial \dot{x}_{i}} = 2\frac{\dot{x}_{i}}{x_{i}} \Longrightarrow \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}_{i}} = 2\frac{[x_{i}\ddot{x}_{i} - \dot{x}_{i}^{2}]}{x_{i}^{2}},$$

$$\frac{\partial \mathcal{L}}{\partial x_{i}} = -\frac{\dot{x}_{i}^{2}}{x_{i}^{2}} + (f^{i} - \bar{f})^{2}$$

$$+2\sum_{k=1}^{n} x_{k} \left(f^{k} - \bar{f}\right) \left(\frac{\partial f^{k}}{\partial x_{i}} - f^{i} - \sum_{j} x_{j} \frac{\partial f^{j}}{\partial x_{i}}\right) + \lambda \quad (12)$$

which gives the Euler-Lagrange equations for i = 1, ..., n as follows:

$$2\ddot{x}_{i} = \frac{\dot{x}_{i}^{2}}{x_{i}} + x_{i} \left(f^{i} - \bar{f} \right)^{2} + 2x_{i} \left[\sum_{k} x_{k} \left(f^{k} - \bar{f} \right) \left(\frac{\partial f^{k}}{\partial x_{i}} - \sum_{j} x_{j} \frac{\partial f^{j}}{\partial x_{i}} \right) \right] + x_{i} \lambda \quad (13)$$

Therefore, λ can be obtained by summing the above equation over i to get:

$$\lambda = \sum_{i} \left[2\ddot{x}_{i} - \frac{\dot{x}_{i}^{2}}{x_{i}} - x_{i} \left(f^{i} - \bar{f} \right)^{2} \right]$$

$$- \sum_{i} \left[2x_{i} \sum_{k} x_{k} \left(f^{k} - \bar{f} \right) \left(\frac{\partial f^{k}}{\partial x_{i}} - \sum_{j} x_{j} \frac{\partial f^{j}}{\partial x_{i}} \right) \right]$$
(14)

Differentiating the replicator equations,

$$\dot{x}_{i} = x_{i} \left(f^{i} - \bar{f} \right) \Longrightarrow
2\ddot{x}_{i} = 2 \left[x_{i} \left(f^{i} - \bar{f} \right)^{2} \right]
+ 2 \left[x_{i} \sum_{k} x_{k} \left(f^{k} - \bar{f} \right) \left(\frac{\partial f^{i}}{\partial x_{k}} - f^{k} - \sum_{j} x_{j} \frac{\partial f^{j}}{\partial x_{k}} \right) \right]
= 2 \left[x_{i} \left(f^{i} - \bar{f} \right)^{2} + x_{i} \sum_{j} x_{k} \left(f^{k} - \bar{f} \right) \left(\frac{\partial f^{i}}{\partial x_{k}} - \sum_{j} x_{j} \frac{\partial f^{j}}{\partial x_{k}} \right) \right]
- 2 \left[x_{i} \sum_{k} x_{k} \left(f^{k} - \bar{f} \right)^{2} \right]$$
(15)

Comparing (13) and (15), we see that the replicator equations (8) satisfy the Euler-Lagrange equations with $\lambda = -2\sum_{k=1}^{n} x_k \left(f^k - \bar{f}\right)^2$. We note that due to the point-wise simplex constraint, the Lagrange multiplier is dependent on the state.

A. Conserved quantity

The Lagrangian \mathcal{L} on the simplex is time-invariant. Hence, there is a conserved quantity E, the energy, which we calculate below. Let $L(x_1, \ldots, x_{n-1}, \dot{x}_1, \ldots, \dot{x}_{n-1})$ denote the Lagrangian \mathcal{L} given in the local coordinates for the simplex x_1, \ldots, x_{n-1} with the understanding that $x_n = 1 - x_1 - \ldots - x_{n-1}$ and $\dot{x}_n = -\dot{x}_1 - \ldots - \dot{x}_{n-1}$. This eliminates the term containing the Lagrange multiplier λ in \mathcal{L} and we get:

$$L = \sum_{k=1}^{n} \left[\frac{\dot{x}_{k}^{2}}{x_{k}} + x_{k} \left(f^{k} - \bar{f} \right)^{2} \right]$$
 (16)

Therefore,

$$E = \sum_{i=1}^{n} \dot{x}_i \frac{\partial L}{\partial \dot{x}_i} - L$$

$$= \sum_{i=1}^{n} \frac{\dot{x}_i^2 - x_i^2 \left(f^i - \bar{f} \right)^2}{x_i} = \text{constant.}$$
(17)

If $\dot{x}_i = x_i (f^i - \bar{f})$ for i = 1, ..., n, we get:

$$E = \sum_{i=1}^{n} \frac{x_i^2 (f^i - \bar{f})^2 - x_i^2 (f^i - \bar{f})^2}{x_i} = 0.$$
 (18)

Thus, solutions to the replicator dynamics are confined to the zero level set of energy. The converse statement is not necessarily true. This can be seen by interpreting the conserved quantity in terms of the FRS inner product of the tangent vectors \dot{x} and $v = [v_1 \dots v_n]$ where $v_k = x_k \left(f^k - \bar{f} \right)$, both of whose components necessarily sum to zero in the simplex. That is,

$$E = \langle \dot{x}, \dot{x} \rangle_{FRS} - \langle v, v \rangle_{FRS} = 0$$

$$\therefore E = 0, x \in \Delta^{n-1} \implies ||\dot{x}||_{FRS} = ||v||_{FRS}$$
 (19)

which does not imply $\dot{x} = v$.

B. The Hamiltonian function

For an equivalent representation of the Euler-Lagrange equations in the co-tangent bundle $T^*\Delta^{n-1}$, following the standard route, we define the momentum variables $p_i, i = 1, ..., n-1$ as follows:

$$p_{i} = \frac{\partial L}{\partial \dot{x}_{i}} = 2\frac{\dot{x}_{i}}{x_{i}} + 2\frac{\sum_{k=1}^{n-1} \dot{x}_{k}}{1 - \sum_{k=1}^{n-1} x_{k}}, 1 \le i \le n - 1$$
 (20)

or equivalently

$$p = 2\tilde{G}(x_1, \dots, x_n)\dot{x}, \text{ where }$$

$$\tilde{G} = [\tilde{g}_{ij}], 1 \le i, j \le n - 1, \quad \tilde{g}_{ij} = \delta_{ij} \frac{2}{x_i} + \frac{2}{1 - \sum_{k=1}^{n-1} x_k}. \quad (21)$$

Note that $\tilde{G}(x)$ is the Fisher-Rao-Shahshahani metric expressed in local coordinates for the simplex. This leads us to define the Hamiltonian function H(x,p) via the Legendre transform. Although this requires $\tilde{G}(x_1,\ldots,x_{n-1})$ to be invertible in the interior of Δ^{n-1} , we are assured of this due to the fact that the metric in local coordinates for the positive orthant restricted to the simplex, $G = diag\left(\frac{1}{x_1},\ldots,\frac{1}{x_n}\right)$ is invertible in $int(\Delta^{n-1})$. Suppressing the arguments of \tilde{G} , we get the Hamiltonian:

$$H(x_1, \dots, x_{n-1}, p) = \frac{1}{2} p^T \tilde{G}^{-1} p - L(x_1, \dots, x_{n-1}, \tilde{G}^{-1} p)$$

= $\frac{1}{4} p^T \tilde{G}^{-1} p + V(x_1, \dots, x_{n-1})$ (22)

where $p = [p_1 \ p_2 \ \dots \ p_{n-1}]^T$. Let $y = [x_1 \ \dots \ x_{n-1}]^T$. Then, Hamilton's equations are:

$$\dot{y} = \frac{\partial H}{\partial p} = \frac{1}{2}\tilde{G}^{-1}(y)p$$

$$\dot{p} = -\frac{\partial H}{\partial y} = g(y, p) - \frac{\partial V(y)}{\partial y}$$
(23)

where g(y,p) is a $n-1 \times 1$ vector whose components are given by $g_i(y,p) = -\frac{1}{4} \frac{\partial p^T \tilde{G}^{-1}(y) p}{\partial y_i} = -\frac{1}{4} p^T \frac{\partial \tilde{G}^{-1}(y)}{\partial y_i} p, i = 1, \dots, n-1.$

We observe that in this dynamics, the state equation contains terms linear in p, whereas the momentum equation comprises terms that are quadratic in p. Therefore, $g_i(y, p) = g_i(y, -p)$. This suggests investigating periodic orbits in level sets of H using Birkhoff's theorem. We define the notion of involutivity and F – reversibility of vector fields under a map $F: M \to M$, following [14].

Definition 2.2. (*Involution*). A diffeomorphism $F: M \to M$ from a manifold M to itself is said to be an involution if $F \neq id_M$, the identity diffeomorphism, and $F^2 = id_M$, i.e. $F(F(m)) = m, \forall m \in M$.

Definition 2.3. (F - reversibility). A vector field X defined over a manifold M is said to be F -reversible, if there exists an involution F such that: $F_*(X) = X$; i.e. F maps orbits of X to orbits of X, reversing the time parametrization. Here $(F_*(X))(m) = (DF)_{F^{-1}(m)}X(F^{-1}(m)) \ \forall \ m \in M$ is the push-forward of X(m). We call F the reverser of X.

Theorem 2.4. (G. D. Birkhoff [15]). Let X be a F-reversible vector field on M and Σ_F the fixed-point set of the reverser F. If an orbit of X through a point of Σ_F intersects Σ_F in another point, then it is periodic.

We refer to [14] for a proof of Birkhoff's theorem. The reverser F in our problem is defined in the proposition below.

Proposition 2.5. The vector field defined by the Hamiltonian dynamics (23) is F-reversible, with the map F given by F(y,p) = (y,-p).

Proof. Let the Hamiltonian vector field in (23) be denoted X_H . We note that F is an involution since $F^2(y,p) = F(y,-p) = (y,p)$. We calculate the pushforward of F as follows:

$$(F_*(X_H))(y,p) = (DF)_{F^{-1}(y,p)}X(F^{-1}(y,p))$$

$$= \begin{bmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & -\mathbb{1} \end{bmatrix} \begin{bmatrix} -\frac{1}{2}\tilde{G}^{-1}(y)p \\ g(y,-p) - \frac{\partial V(y)}{\partial y} \end{bmatrix}$$

$$= -\begin{bmatrix} \frac{1}{2}\tilde{G}^{-1}(y)p \\ g(y,p) - \frac{\partial V(y)}{\partial y} \end{bmatrix} = -X_H(y,p) \tag{24}$$

where $\mathbb{O},\mathbb{1}$ are respectively n-1 dimensional zero and identity matrices.

We are now ready to state a theorem on the existence of periodic orbits for the Hamiltonian dynamics (23) in the special case n=2 corresponding to the 1- dimensional simplex.

Theorem 2.6. Consider the Hamiltonian system defined on $M = \{(y, p) : y = [x_1 \dots x_{n-1}], x \in int(\Delta^{n-1}), p \in \mathbb{R}^{n-1}\}$, and a frequency dependent fitness $f(x) \in \mathbb{R}^n$ such that the Hamiltonian function is given as

$$H(y, p) = T(y, p) + V(y)$$
 (25)

where the kinetic energy term is $T(y,p) = \frac{1}{4} p^T \tilde{G}^{-1}(y) p$ and the potential energy term is $V(y) = -\sum_{k=1}^{n-1} y_k \left(f^k(y) - \bar{f} \right)^2 - \left(1 - \sum_{k=1}^{n-1} y_k \right) \left(f^n(y) - \bar{f} \right)^2$ with the Hamilton's equations given by (23). For the case n=2, the level sets of H are 1- dimensional in phase space. Assuming that for a fixed c the level set has one connected component, then for c<0, the trajectory of this dynamics is a periodic orbit if the nonlinear equation V(y)=c has two distinct solutions for

Proof. Consider the map $F: M \to M$ such that F(y,p) = (y,-p). By proposition 2.5, the Hamiltonian vector field is reversible with F as the reverser. Next, we note that the fixed point set of the map is

 $y \in int(\Delta^1)$.

$$\Sigma_F = \{(y, p) : y = [x_1 \dots x_{n-1}], x \in int(\Delta^{n-1}), p = 0\}$$
 (26)

To find the intersections of orbits in $H(t) \equiv c \neq 0$, with Σ_F , we substitute p=0 in the Hamiltonian to get V(y)=c. In the case n=2, the connectivity assumption means that a level set is an orbit. If the equation V(y)=c has two distinct roots in $int(\Delta^1)$, the orbits in the level sets of the Hamiltonian intersect Σ_F twice. It follows from Birkhoff's theorem that such orbits are periodic.

III. THE HAMILTONIAN DYNAMICS FOR n = 2

We specialize to the case when n = 2. The 1-dimensional simplex has local coordinate x_1 . Consider the Lagrangian for a linear fitness f = Ax, where $A = [a_{ij}], 1 \le i, j \le 2$ expressed as follows:

$$L = \frac{\dot{x}_1^2}{x_1} + \frac{\dot{x}_2^2}{x_2} + x_1 \left((Ax)^1 - x^T Ax \right)^2 + x_2 \left((Ax)^2 - x^T Ax \right)^2$$

$$= \dot{x}_1^2 \left(\frac{1}{x_1} + \frac{1}{1 - x_1} \right) + x_1 (1 - x_1)^2 \left((Ax)^1 - (Ax)^2 \right)^2$$

$$+ (1 - x_1)x_1^2 \left((Ax)^1 - (Ax)^2 \right)^2$$

$$= \frac{\dot{x}_1^2}{x_1 (1 - x_1)} + x_1 (1 - x_1) \left((Ax)^1 - (Ax)^2 \right)^2$$
(27)

In simplifying these calculations, we have used the following relationships: $x_1 (f^1 - \bar{f})^2 = x_1 (1 - x_1)^2 (f^1 - f^2)^2$ and

 $(1-x_1)\left(f^2-\bar{f}\right)^2=x_1^2(1-x_1)\left(f^1-f^2\right)^2$. The momentum variable p_1 is defined as

$$p_1 = \frac{\partial L}{\partial \dot{x}_1} = \frac{2\dot{x}_1}{x_1(1 - x_1)}.$$
 (28)

which can be inverted in $int(\Delta^1)$ to obtain \dot{x}_1 in terms of x_1, p_1 . The Hamiltonian H is given as follows:

$$H(x_1, p_1) = \frac{p_1^2 x_1 (1 - x_1)}{2} - \frac{\left(p_1^2 x_1^2 (1 - x_1)^2\right)}{4x_1 (1 - x_1)}$$
$$-x_1 (1 - x_1) \left((Ax)^1 - (Ax)^2\right)^2$$
$$= \frac{p_1^2 x_1 (1 - x_1)}{4} - x_1 (1 - x_1) \left((Ax)^1 - (Ax)^2\right)^2$$
(29)

so that the Hamiltonian dynamics is given as:

$$\dot{x}_{1} = \frac{\partial H}{\partial p_{1}} = \frac{p_{1}x_{1}(1 - x_{1})}{2}
\dot{p}_{1} = -\frac{\partial H}{\partial x_{1}} = -\frac{p_{1}^{2}(1 - 2x_{1})}{4} + (1 - 2x_{1})(ax_{1} + b)^{2}
+ 2ax_{1}(1 - x_{1})(ax_{1} + b)$$
(30)

where $a = a_{11} - a_{21} - a_{12} + a_{22}$, $b = a_{12} - a_{22}$. The trajectories in the simplex corresponding to the zero level set of the Hamiltonian are given by the replicator dynamics (8), upto a time scale change. This can be verified by setting H = 0 and noting that the momentum variable satisfies the following relationship:

$$p_{1} = \pm 2 \left[\left((Ax)^{1} - (Ax)^{2} \right) \right]$$

$$= \pm 2 \left[(a_{11} - a_{21}) x_{1} + (a_{12} - a_{22}) (1 - x_{1}) \right] \Longrightarrow$$

$$\dot{x}_{1} = \pm x_{1} \left((Ax)^{1} - x^{T} Ax \right)$$
(31)

A. Non-zero level sets of the Hamiltonian

Suppose p(0) is such that $H(x_1, p_1) \equiv c \neq 0$, $a = a_{11} - a_{21} - a_{12} + a_{22}$ and $b = a_{12} - a_{22}$. Then, the momentum variable can be given explicitly in terms of the state x_1 as follows:

$$p_1 = \pm 2\sqrt{\frac{x_1(1-x_1)(ax_1+b)^2+c}{x_1(1-x_1)}}$$
 (32)

where c = H(0). For this case, we show the existence of periodic orbits in the state-momentum variable space in the following theorem.

Theorem 3.1. Consider the Hamiltonian system defined on $M = \{(x_1, p_1) : x_1 \in (0, 1), p_1 \in \mathbb{R}\}$, and the matrix $A = [a_{ij}]$, $1 \le i, j \le 2$ such that the Hamiltonian function is given as

$$H(x_1, p_1) = \frac{p_1^2 x_1 (1 - x_1)}{4} - x_1 (1 - x_1) \left((Ax)^1 - (Ax)^2 \right)^2$$
(33)

with the corresponding dynamics

$$\dot{x}_{1} = \frac{\partial H}{\partial p_{1}} = \frac{p_{1}x_{1}(1 - x_{1})}{2}
\dot{p}_{1} = -\frac{\partial H}{\partial x_{1}} = -\frac{p_{1}^{2}(1 - 2x_{1})}{4} + (1 - 2x_{1})\left((Ax)^{1} - (Ax)^{2}\right)^{2}
+ 2ax_{1}(1 - x_{1})\left((Ax)^{1} - (Ax)^{2}\right)$$
(34)

where $x = [x_1 \ 1 - x_1]^T$. Then, the trajectories of this dynamics in the non-zero level sets of the Hamiltonian function consist of periodic orbits if the polynomial

$$[-a^{2}]z^{4} + [a^{2} - 2ab]z^{3} + [-b^{2} + 2ab]z^{2} + [b^{2}]z + c = 0$$
 (35)

with $a = a_{11} - a_{21} - a_{12} + a_{22}$, $b = a_{12} - a_{22}$, c = H(0) has two distinct roots in $int(\Delta^1)$.

Proof. Consider the map $F: M \to M$ defined in proposition 2.5. We have shown that the Hamiltonian vector field is F-reversible. The fixed point set Σ_F of the map F is the set of all points in M satisfying $p_1 = 0$. To apply Birkhoff's theorem, we investigate the number of intersections of trajectories in the level set $H(t) \equiv c$ with Σ_F by solving for x_1 such that $p_1 = 0$. Setting $p_1 = 0$ in (32) is equivalently

$$x_1(1-x_1)[ax_1+b]^2+c=0$$
(36)

Simplifying (36), we see that Birkhoff's condition is equivalent to the following equation having two distinct roots in the interior of the simplex:

$$[-a^{2}]z^{4} + [a^{2} - 2ab]z^{3} + [-b^{2} + 2ab]z^{2} + [b^{2}]z + c = 0$$
 (37)

with $a = a_{11} - a_{21} - a_{12} + a_{22}$, $b = a_{12} - a_{22}$, c = H(0). This concludes the proof.

There may exist trajectories for the Hamiltonian dynamics other than periodic orbits. The equilibria for this dynamics

$$\dot{x}_1^* = 0 \implies x_1^* = 0, 1 \text{ or } p_1^* = 0.$$

$$\dot{p}_1^* = 0 \implies (1 - 2x_1^*) \left[\frac{(p_1^*)^2}{4} - \left((Ax^*)^1 - (Ax^*)^2 \right)^2 \right]$$

$$-2ax_1^* (1 - x_1^*) \left((Ax^*)^1 - (Ax^*)^2 \right) = 0.$$
(38)

Therefore, $x_1^* = 0$ or 1 gives $p_1^* = \pm 2 \left\lfloor (Ax^*)^1 - (Ax^*)^2 \right\rfloor$. However, since the Hamiltonian is well defined only in the interior of the simplex, we ignore these and consider $p_1^* = 0$. When $p_1^* = 0$, x_1^* are given by solutions in $int(\Delta^{n-1})$ to (38). The simplex is preserved in either case since when $x_1 = 0$ or $x_1 = 1$, $\dot{x}_1 = 0$.

IV. SIMULATION RESULTS

We illustrate the theorem of the previous section using an example. We further simplify the analysis by using the invariance of the difference of fitness components from the average to the addition of a component-wise uniform vector. Let C_i denote the 2×2 matrix whose i^{th} column elements are

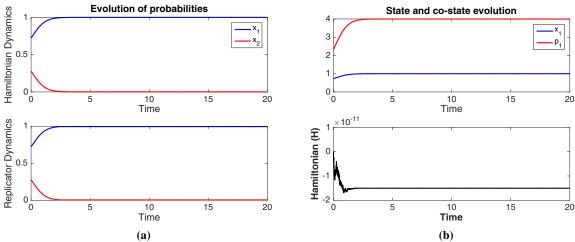


Fig. 1: Coordination game. (a). Simulation of the replicator and Hamiltonian dynamics for $x_1(0)$ uniformly chosen in (0,1) and p(0) initialized in terms of $(x(0),\dot{x}(0))$ to satisfy the replicator dynamics. In this case, the Hamiltonian is zero and the trajectories of both dynamics coincide. x_1 is in blue, x_2 in red. (b). Evolution of the state, co-state and the Hamiltonian. The Hamiltonian is conserved upto an error of the order of 10^{-11} Step size, $\Delta t = 10^{-4}$.

one and others zero. The linear fitness generated by matrices $A = [a_{ij}], 1 \le i, j \le 2$, and $\tilde{A} = (A - a_{21}C_1 - a_{12}C_2)$ satisfy

$$Ax - x^T Ax = \tilde{A}x - x^T \tilde{A}x \tag{39}$$

Therefore, it is sufficient to analyze the Hamiltonian dynamics for the fitness defined by diagonal matrices parametrized by $\xi \in \mathbb{R}$ such as

$$D = \left[\begin{array}{cc} \xi & 0 \\ 0 & 1 \end{array} \right] \tag{40}$$

In correspondence with the parameters a, b defined earlier, we get $a = 1 + \xi$ and b = -1 and the polynomial (37) becomes

$$-(\xi+1)^2z^4 + +(\xi+1)(\xi+3)z^3 - (2\xi+3)x_1^2 + x_1 + c = 0$$
(41)

A. Coordination game

We consider the fitness f = Dx for a coordination game [16] with $\xi = 2$. The numerical simulations of the Hamiltonian system are performed using the mid-point rule [17]. The simulated trajectories of the Hamiltonian dynamics for a random initial condition for $x_1(0)$ and the $p_1(0)$ chosen according to (32) for c = 0 is depicted in Figure 1. As expected, the trajectories of x_1 from the Hamiltonian dynamics coincide with the replicator dynamics and $H(t) \equiv 0$. Simulations for random initialization of $p_1(0)$ fixes the non-zero value of the Hamiltonian c in our calculations. For $\xi = 2$, the equation (41) has two roots real roots in the interval (0,1) taking values 0.9019 and 0.7038 (precision upto the order of 10^{-5}) and two imaginary roots. Hence, the Hamiltonian vector field is F - reversible with the map $F(x_1, p_1) = (x_1, -p_1)$, and has two distinct intersections with the fixed point set Σ_F . Thus, the conditions of Theorem 3.1 are satisfied, resulting in periodic behaviour depicted in Figure 2.

V. CONCLUSIONS AND FUTURE WORK

In this work, we have considered a variational problem on the probability simplex due to Svirezhev. We addressed it from a Hamiltonian point of view, and exploited time-translation symmetry of the Lagrangian and associated conserved quantity. We appealed to Birkhoff's theorem to investigate existence of periodic orbits as solutions to the Hamiltonian dynamics in a special case. We extended Svirezhev's result to general fitness maps and showed that solutions to the replicator dynamics satisfy the Euler-Lagrange equations and hence are extremals of the variational problem. We have presented an illustrative example (arising from a matrix game) on a one-dimensional simplex through numerical simulations. We plan to treat questions of conjugate points for the variational problem in future work.

Introduction of control variables into replicator dynamics lead to other types of optimality principles beyond the ones treated here. Associated Hamiltonian dynamics are under investigation.

REFERENCES

- [1] E. Akin, *The geometry of population genetics*, vol. 31. Springer Science & Business Media, 2013.
- [2] M. Kimura, "On the change of population fitness by natural selection," Heredity, vol. 12, no. 2, p. 145, 1958.
- [3] E. Wei, E. W. Justh, and P. S. Krishnaprasad, "Pursuit and an evolutionary game," in *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, vol. 465, pp. 1539– 1559. The Royal Society. 2009.
- [4] W. Ewens, "An optimizing principle of natural selection in evolutionary population genetics," *Theoretical Population Biology*, vol. 42, no. 3, pp. 333–346, 1992.
- [5] W. J. Ewens and A. Hastings, "Aspects of optimality behavior in population genetics theory," in *Evolution and Biocomputation*, pp. 7– 17, Springer, 1995.
- [6] A. Hastings and G. A. Fox, "Optimization as a technique for studying population genetics equations," in *Evolution and Biocomputation*, pp. 18–26, Springer, 1995.

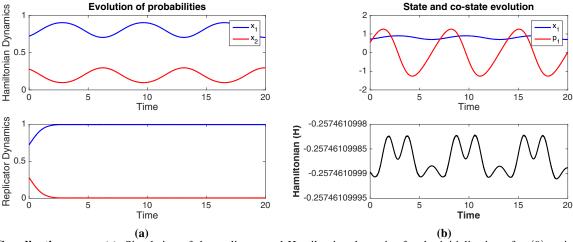


Fig. 2: Coordination game. (a). Simulation of the replicator and Hamiltonian dynamics for the initialization of $x_1(0)$ as in Fig. 1 and p(0) uniformly chosen in (0,1). x_1 is in blue, x_2 in red. x_1 and hence $x_2 = 1 - x_1$ are periodic. (b). Evolution of the state, co-state and the Hamiltonian. x_1, p_1 are periodic solutions. The Hamiltonian is conserved upto an error of the order of 10^{-10} . Step size, $\Delta t = 10^{-4}$.

- [7] Y. M. Svirezhev, "Optimum principles in genetics," *Studies on theoretical genetics*, pp. 86–102, 1972.
- [8] Y. M. Svirezhev and V. P. Passekov, Fundamentals of mathematical evolutionary genetics, vol. 22. Springer Science & Business Media, 2012.
- [9] P. J. Schoemaker, "The quest for optimality: A positive heuristic of science?," *Behavioral and Brain Sciences*, vol. 14, no. 2, pp. 205–215, 1991
- [10] P. D. Taylor and L. B. Jonker, "Evolutionary stable strategies and game dynamics," *Mathematical biosciences*, vol. 40, no. 1-2, pp. 145–156, 1978.
- [11] S. Shahshahani, A new mathematical framework for the study of linkage and selection. American Mathematical Soc., 1979.
- [12] J. Hofbauer and K. Sigmund, Evolutionary games and population dynamics. Cambridge university press, 1998.
- [13] V. Raju and P. S. Krishnaprasad, Lie algebra of fitness and replicator control. To be submitted.
- [14] M. Mischiati and P. S. Krishnaprasad, "The dynamics of Mutual Motion Camouflage," *Systems & Control Letters*, vol. 61, pp. 894–903, sep 2012.
- [15] G. D. Birkhoff, "The restricted problem of three bodies," *Rendiconti del Circolo Matematico di Palermo (1884-1940)*, vol. 39, no. 1, p. 265, 1915.
- [16] J. W. Weibull, Evolutionary game theory. MIT press, 1997.
- [17] M. A. Austin, P. S. Krishnaprasad, and L.-S. Wang, "Almost poisson integration of rigid body systems," *Journal of Computational Physics*, vol. 107, no. 1, pp. 105–117, 1993.